Enhancement of nuclear Schiff moments and time reversal violation in atoms due to combination of soft nuclear octupole and quadrupole vibrations

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Nuclear forces violating parity and time reversal invariance ($\mathcal{P},\mathcal{T}$-odd) produce $\mathcal{P},\mathcal{T}$-odd nuclear moments, for example, the nuclear Schiff moment. In turn, this moment can induce the electric dipole moment (EDM) in the atom. The contribution to the Schiff moment from the soft collective quadrupole and octupole vibrations in spherical nuclei is calculated in the framework of the quasiparticle random phase approximation with separable quadrupole and octupole forces. The values of nuclear Schiff moments predicted for odd $^{217-221}$Ra and $^{217-221}$Ra isotopes indicate a possibility of enhancement by a factor of 50 or more as compared to the experimentally studied spherical nuclei ^{199}Hg and ^{129}Xe. Since the EDM in very heavy atoms, such as Ra, Rn, and Fr, has an additional enhancement rapidly increasing with nuclear charge Z, the EDM enhancement can exceed two orders of magnitude. We discuss the nuclear structure effects causing an enhancement of the Schiff moment.

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I. INTRODUCTION

The search for interactions violating time reversal ($\mathcal{T}$-) invariance is an important part of studies of fundamental symmetries in nature. The manifestations of $\mathcal{CP}$-violation (and therefore, through the $\mathcal{CPT}$-theorem, of $\mathcal{T}$-invariance) in systems of neutral K- and B-mesons [1] set limits on physical effects beyond the standard model. However, the main hopes for the extraction of nucleon-nucleon and quark-quark interactions violating fundamental symmetries emerge from the experiments with atoms and atomic nuclei, see the recent review [2] and references therein. For example, the best limits on $\mathcal{P},\mathcal{T}$-odd forces have been obtained from the measurements of the atomic electric dipole

moment (EDM) in the ^{199}Hg [3] and ^{129}Xe [4] nuclei. As we know from past experience with $\mathcal{P}$-odd forces, see the review article [5], there are powerful many-body mechanisms in heavy atoms and nuclei which allow one to expect a significant amplification of effects generated on the level of elementary interactions. There are also suggestions for using possible molecular and solid state enhancement mechanisms [6, 7, 8].

The theoretical calculation of atomic EDM proceeds through the *nuclear Schiff moment* $\mathbf{S}$ since the nuclear EDM is shielded by atomic electrons [9]. The Schiff moment produces the $\mathcal{PT}$-odd electrostatic potential that, in turn, induces the atomic EDM. The expectation value of the vector operator $\mathbf{S}$ in a stationary nuclear state characterized by certain quantum numbers of angular momentum, JM, is possible only for $J \neq 0$ owing to the requirements of rotational invariance. Since all even-even nuclei have zero ground state spin, we need to consider an odd-A nucleus. Furthermore, the non-zero expectation value of a polar vector $\mathbf{S}$ requires parity non-conservation in a nucleus; in addition, being proportional to the $\mathcal{T}$-odd pseudoscalar $\langle(\mathbf{S}\cdot\mathbf{J})\rangle$, this expectation value reveals the violation of $\mathcal{T}$-invariance.

A reliable evaluation of the nuclear Schiff moment should include the estimates of renormalization effects due to "normal" strong interactions inside the nucleus. The core polarization by the odd nucleon is important, especially in the case of the odd neutron, as ^{199}Hg and ^{129}Xe. Calculations [10, 11, 12] show that the resulting configuration mixing, depending on details of the method, may change the result of the independent particle model by a factor of about 2. A possibility of using accidental proximity of nuclear levels with the same spin and opposite parity was pointed out in Refs. [9, 13]. In such approaches, possible *coherent* enhancement mechanisms are usually not considered.

The statistical many-body enhancement of parity non-conservation in the region of the high level density of neutron resonances was predicted theoretically (see e.g. reviews [5, 14] and references therein). The existence of such enhancement is now well documented experimentally [15]. The simultaneous violation of parity and time reversal invariance can be enhanced by the firmly established $\mathcal{P}$-violation due to $\mathcal{P}$-odd $\mathcal{T}$-even weak interactions. The idea of a possible role of *static octupole deformation* [14, 16, 17, 18] exploited the parity doublets which appear in the presence of pear-shaped intrinsic deformation of the mean field. The doublet partners have similar structure and relatively close energies so that they can be more effectively mixed by $\mathcal{P}$-odd forces. The Schiff moment in the body-fixed frame is enhanced being in fact proportional to the collective octupole moment. The microscopic calculations [19, 20] predict a resulting Schiff moment by two-three orders of magnitude greater than in spherical nuclei; this enahncement was confirmed in Refs.

[21, 22]. The uncertainties related to the specific assumptions on $\mathcal{PT}$-odd forces and different approximations for nuclear structure are on the order of a factor 2 for the resulting Schiff moment.

It was suggested in Ref. [23] that *soft octupole vibrations* observed in some regions of the nuclear chart more frequently than static octupole deformation may produce a similar enhancement of the Schiff moment. This would make heavy atoms containing nuclei with large collective Schiff moments attractive for future experiments in search for $\mathcal{P},\mathcal{T}$-violation; experiments of this type are currently under progress or in preparation in several laboratories. Recently we performed [24] the estimate of the Schiff moment generated in nuclei with the soft octupole mode and showed that the result is nearly the same as in the case of the static octupole deformation.

A related idea is explored in the present paper. It is known that some nuclei are soft with respect to *both quadrupole and octupole* modes, see for example recent predictions for radioactive nuclei along the $N = Z$ line [25]. The light isotopes of Rn and Ra are spherical but with a soft quadrupole mode and therefore large amplitude of quadrupole vibrations. The spectra of these nuclei display long quasivibrational bands [26] based on the ground state and on the octupole phonon, with positive and negative parity, respectively. These bands are connected via low-energy electric dipole transitions. This situation seems to be favorable for the enhancement of $\mathcal{P},\mathcal{T}$-odd effects.

Below we show that the enhancement indeed exists in spherical nuclei which have both collective quadrupole and octupole modes. The main mixing occurs between the levels of the same spin and opposite parity that carry a significant admixture of the 2^+ or/and 3^- phonons to the odd nucleon. In the odd-neutron nuclei the Schiff moment is originated by the proton contribution to the collective phonon. A number of such nuclei have an appropriate opposite parity level with the same angular momentum close to ground state. In this case the enhancement factor for the nuclear Schiff moment and atomic EDM may exceed 50. At the next stage the task of theory should be to combine all effects generated by $\mathcal{PT}$-violating interaction, including core polarization and weak interaction admixtures to the phonon structure.

II. COLLECTIVE SCHIFF MOMENT IN SPHERICAL NUCLEI: A SIMPLE ESTIMATE

Consider a nucleus with two close levels of the same spin J and opposite parity, ground state $|\text{g.s.}\rangle$ and excited state $|x\rangle$. The energies of these states are $E_{\text{g.s.}}$ and E_x, respectively. Let W be a $\mathcal{P},\mathcal{T}$-odd interaction mixing the unperturbed states. Assuming that the mixing matrix elements of $\mathbf{S}$ and W are real, we can write down the Schiff moment emerging in the actual mixed ground

state as

$$\mathbf{S} = 2\frac{\langle \text{g.s.}|W|x\rangle\langle x|\mathbf{S}|\text{g.s.}\rangle}{E_{\text{g.s.}} - E_x}. \tag{1}$$

However, as it was explained in Ref. [9], in the case of mixing of close *single-particle* states one should not expect a large enhancement. For example, in a simple approximate model, where the strong nuclear potential is proportional to nuclear density and the spin-orbit interaction is neglected, the matrix element $\langle \text{g.s.}|W|x\rangle$ contains the single-particle momentum operator. This matrix element is proportional to $(E_{\text{g.s.}} - E_x)$, so that the small energy denominator cancels out. As mentioned above, the collective Schiff moments in nuclei with static octupole deformations may be by 2-3 orders of magnitude stronger than single-particle moments in spherical nuclei.

The mechanism generating the *collective* Schiff moment in spherical nuclei might be the following [24] (we illustrate the idea by an example). Let an odd-A nucleus have the unperturbed ground state of spin J built as a zero spin core plus an unpaired nucleon in the spherical mean field orbit with angular momentum $j = J$. The interaction between the odd particle and vibrations of the core causes an admixture of a quadrupole phonon to the ground state if the nuclear spin $J > 1/2$:

$$|\text{g.s.}\rangle = a_0|j = J\rangle + a_2|[j, 2^+]_J\rangle. \tag{2}$$

An opposite parity state can be formed by adding an octupole phonon to the ground state particle,

$$|x >= |[j, 3^-]_J\rangle. \tag{3}$$

To find the $\mathcal{P},\mathcal{T}$-odd Schiff moment (1) we need to know the matrix elements of the $\mathcal{P},\mathcal{T}$-odd nucleon-nucleon interaction. To the first order in the non-relativistic nucleon velocity p/m, the $\mathcal{P},\mathcal{T}$-odd interaction can be presented as [9]

$$W_{ab} = \frac{G}{\sqrt{2}}\frac{1}{2m}\Big((\eta_{ab}\boldsymbol{\sigma}_a - \eta_{ba}\boldsymbol{\sigma}_b)\cdot\boldsymbol{\nabla}_a\delta(\mathbf{r}_a - \mathbf{r}_b) + \eta'_{ab}\,[\boldsymbol{\sigma}_a \times \boldsymbol{\sigma}_b]\cdot\{(\mathbf{p}_a - \mathbf{p}_b), \delta(\mathbf{r}_a - \mathbf{r}_b)\}\Big), \tag{4}$$

where $\{\ ,\ \}$ is an anticommutator, G is the Fermi constant of the weak interaction, m is the nucleon mass, and $\boldsymbol{\sigma}_{a,b}$, $\mathbf{r}_{a,b}$, and $\mathbf{p}_{a,b}$ are the spins, coordinates, and momenta, respectively, of the interacting nucleons a and b. The dimensionless constants η_{ab} and η'_{ab} characterize the strength of the $\mathcal{P},\mathcal{T}$-odd nuclear forces; in fact, experiments on measurement of the EDMs are aimed at extracting the values of these constants.

A single-particle matrix element of W has been estimated in Ref. [20]. Based on this experience, we present the matrix elements of W between the states (2) and (3) dressed by the phonons as

single-particle matrix elements times numerical factors K_W.

$$\langle \text{g.s.}|W|x\rangle = \eta \frac{G}{2\pi\sqrt{2}mr_0^4 A^{1/3}} K_W \approx \frac{\eta}{A^{1/3}} K_W \text{ eV}; \tag{5}$$

here $r_0 \approx 1.2$ fm is an internucleon distance, and A is the mass number of the nucleus. By definition, $K_W \approx 1$ for single-particle matrix elements. Numerical calculations show that for the phonon-dressed close opposite parity states $K_W \approx 0.3$.

Similarly, we can present the matrix elements of the Schiff moment operator S between the phonon-dressed states as single-particle matrix elements times numerical factors K_S,

$$\langle \text{g.s.}|S_z|x\rangle = K_S\, e \cdot \text{fm}^3. \tag{6}$$

Realistically, single-particle matrix elements K_S are between 0.3 and 2 when defined for the maximum projection J_z of the angular momentum J. Numerical calculations has shown that for the phonon-dressed close opposite parity states $K_S \approx 1.0$. Although there is an enhancement of the Schiff moment matrix element between the quadrupole and octupole phonon states (enhancement factor ~ 2), that has a collective origin, the fragmentation of quasiparticle-phonon components and angular momentum recoupling reduce this factor typically to $K_S \approx 1.0$.

In the case of *static* deformation, in the "frozen" body-fixed frame the intrinsic collective Schiff moment S_{intr} of the deformed nucleus can exist without any $\mathcal{P},\mathcal{T}$-violation [19, 20]

$$S_{\text{intr}} \approx \frac{9}{20\pi\sqrt{35}}\, eZR^3\beta_2\beta_3 = \frac{3}{5\sqrt{35}} O_{\text{intr}}\beta_2 \;, \tag{7}$$

where β_2 is the static quadrupole and β_3 is the static octupole deformation parameters, O_{intr} is the static octupole moment. Of course, in the space-fixed laboratory frame, the nucleus has definite angular momentum rather than fixed orientation, and this makes the expectation value of the Schiff moment to vanish in the case of no $\mathcal{PT}$-violation.

The relation (7) should hold [24] for the *dynamic* quadrupole and octupole deformations in systems with spherical equilibrium shape. Using eqs. (1,5), and (6) we can find the ground state Schiff moment:

$$S = \frac{\eta}{E_{\text{g.s.}} - E_x} \frac{G}{\pi\sqrt{2}mr_0^4 A^{1/3}} K_W K_S\, e \cdot \text{fm}^3 \approx 10^{-5}\eta \frac{100\text{ keV}}{E_{\text{g.s.}} - E_x} \frac{2K_S K_W}{A^{1/3}}\, e\,\text{fm}^3. \tag{8}$$

For both single-particle matrix elements and collective matrix elements between the phonon states $K_S K_W \approx 0.3$. Therefore, in the case of close levels of opposite parity ($E_{\text{g.s.}} - E_x \sim 100$ keV), the Schiff moment exceeds that of ^{199}Hg by two orders of magnitude:

$$S \approx 100 \cdot 10^{-8}\eta \frac{100\text{ keV}}{E_{\text{g.s.}} - E_x}\, e\,\text{fm}^3 \sim 70\; S(^{199}\text{Hg}). \tag{9}$$

Here we used the Schiff moment value from Ref. [27], $S(^{199}\mathrm{Hg}) = -1.4 \cdot 10^{-8} \eta\, e \cdot \mathrm{fm}^3$.

Below we give the details of the calculations in the framework of QRPA for quadrupole and octupole phonons.

III. DESCRIPTION OF CALCULATIONS

A. QRPA phonons and particle-phonon interaction

We start with the quadrupole ($J^\pi = 2^+$) and octupole ($J^\pi = 3^-$) phonon states in even-even nuclei based on a conventional model Hamiltonian,

$$H = H_{\mathrm{s-p}} + H_{\mathrm{pair}} + H_{\mathrm{phon}}. \tag{10}$$

The first term, $H_{\mathrm{s-p}}$, describes the Woods-Saxon potential. The following parameterization was used:

$$V_c^{p(n)} = -49.6 \left(1 + (-) 0.86 \, \frac{N - Z}{A} \right) \mathrm{MeV}$$

and

$$V_{ls} = 18.8 \left(\frac{A}{A - 1} \right)^2 \mathrm{MeV}$$

are the strength parameters for the central and spin-orbital potentials, respectively; $R = 1.3\, A^{1/3}$ fm and $a = 0.7$ fm are the radius and diffuseness parameters. The second term, H_{pair}, is pairing interaction with the pairing strength

$$G_p = \frac{17.9 + 0.176\, (N - Z)}{A}$$

for protons and

$$G_n = \frac{18.95 - 0.078\, (N - Z)}{A}$$

for neutrons. The BCS formalism was used that yields a quasiparticle basis with corresponding Bogoliubov transformation coefficients u_j and v_j. The last term, H_{phon}, presents RPA phonons obtained with a separable multipole-multipole interaction,

$$H_{\mathrm{phon}} = \sum_{\lambda\mu} \omega_\lambda Q^\dagger_{\lambda\mu} Q_{\lambda\mu}. \tag{11}$$

The building blocks of the model are the two-quasiparticle RPA phonons,

$$Q^\dagger_{\lambda,\mu} = \frac{1}{2} \sum_{j_1, j_2} \left[A^\lambda_{j_1, j_2} [\alpha^\dagger_{j_1} \alpha^\dagger_{j_2}]_{\lambda,\mu} - (-)^{\lambda-\mu} B^\lambda_{j_1, j_2} [\alpha_{j_1} \alpha_{j_2}]_{\lambda,\mu} \right], \tag{12}$$

where A_{j_1,j_2} and B_{j_1,j_2} are the forward and backward phonon amplitudes,

$$A^{\lambda}_{j_1,j_2} = \frac{1}{\sqrt{2Z(\lambda)}} \frac{f^{\lambda}(j_1 j_2) u^{(+)}_{j_1,j_2}}{\varepsilon(j_1,j_2) - \omega_\lambda}; \quad B^{\lambda}_{j_1,j_2} = \frac{1}{\sqrt{2Z(\lambda)}} \frac{f^{\lambda}(j_1 j_2) u^{(+)}_{j_1,j_2}}{\varepsilon(j_1,j_2) + \omega_\lambda}, \tag{13}$$

where $Z(\lambda)$ is a normalization factor, $f^{\lambda}(j_1 j_2) =< j_1 || r^{\lambda} Y_{\lambda,\mu} || j_2 >$, and coherence factors of the Bogoliubov canonical transformation are $u^{(\pm)}_{1,2} = u_1 v_2 \pm v_1 u_2$ and $v^{(\pm)}_{1,2} = u_1 u_2 \pm v_1 v_2$.

The phonon frequencies ω_λ are the roots of the characteristic RPA equations for each multipolarity λ,

$$X(\lambda) \equiv \frac{1}{2\lambda+1} \sum_{j_1,j_2} \frac{[f^{\lambda}(j_1 j_2) u^{(+)}_{j_1,j_2}]^2 \varepsilon(j_1,j_2)}{\varepsilon^2(j_1,j_2) - \omega^2_\lambda} = \frac{1}{\chi(\lambda)}, \tag{14}$$

where $\chi(\lambda)$ is the strength parameter and $\varepsilon(j_1,j_2) = \varepsilon(j_1) + \varepsilon(j_2)$ is the unperturbed two-quasiparticle energy. Solving these equations one obtains the energies of the phonons and internal structure of the phonon operator (12) hidden in the amplitudes of different two-quasiparticle components. The values of the strength parameters, $\chi(2) = 0.0187$ and $\chi(3) = 0.0019$, were chosen to reproduce the excitation energies of the $J^\pi = 2^+_1$ and the $J^\pi = 3^-_1$ states in $^{212-218}$Ra and Rn isotopes.

Since we are interested in the evaluation of the Schiff moment of the odd-neutron nuclei, the second step of calculations reduces to the solution of the secular equation for the odd-A nucleus with the even-even core excitations described above. If we neglect the quasiparticle+two-phonon components in the wave function of an excited state of an odd-A nucleus, then the corresponding wave function has the following form:

$$\Psi_n(J^\pi) = C_J \Big(\alpha^\dagger_{JM} + \sum_{\lambda,j} D^{\lambda,n}_{Jj} [\alpha^\dagger_j \otimes Q^+(\lambda)]_{JM} \Big) \Psi_0. \tag{15}$$

The energy $E_n(J)$ of the $n^{\rm th}$ state with angular momentum J in the odd-mass nucleus, the amplitudes of the quasiparticle-phonon components,

$$D^{\lambda,n}_{Jj} = \sqrt{\frac{2\lambda+1}{(2J+1)2Z(\lambda)}} \frac{f^{\lambda}(Jj) v^{(-)}_{J,j}}{\varepsilon(j) + \omega_\lambda - E_n}, \tag{16}$$

and the amplitude of the single-quasiparticle component,

$$C^{-2}_{J,n} = 1 + \sum_{\lambda,j} (D^{\lambda,n}_{Jj})^2, \tag{17}$$

are obtained from the solution of the following secular equation [28]:

$$\varepsilon(J) - E_n = \sum_{\lambda,j} \left(D^{\lambda,n}_{Jj} \right)^2 [\varepsilon(j) + \omega_\lambda - E_n]. \tag{18}$$

The quasiparticle-phonon structures of the wave functions for the odd-neutron radium and radon isotopes with A=217, 219 and 221 are shown in Table I.

B. Calculation of the Schiff Moment

Having determined the wave-functions one may proceed with the calculation of the Schiff moment according to the Eq. (1), where for the ground state we will use notation J_g^π and for the first excited state of opposite parity $J_g^{-\pi}$:

$$S(J_g^\pi) = 2\,\frac{\langle J_g^\pi|W|J_g^{-\pi}\rangle\langle J_g^{-\pi}J_g|S_z|J_g^\pi J_g\rangle}{E(J_g^\pi)-E(J_g^{-\pi})}, \tag{19}$$

where W is the $\mathcal{P},\mathcal{T}$-violating nucleon-nucleon interaction given by the Eq. (4) and $\langle J_g^{-\pi}J_g|S|J_g^\pi J_g\rangle$ is the matrix element of the Schiff operator $\mathbf{S}$,

$$S_\mu = \frac{1}{10}\sqrt{\frac{4\pi}{3}}\sum_i Y_{1\mu}(\theta_i,\varphi_i)e_i\left[r_i^3-\frac{5}{3Z}\,r_{\rm ch}^2 r_i\right], \tag{20}$$

with the maximum projection $M=J_g$ of angular momentum and $r_{\rm ch}^2$ is the mean square charge radius.

Since only the proton components of the phonons contribute to the matrix element of the Schiff moment, this matrix element for the case of the odd neutron can be written as

$$\langle J_g^\pm J_g|S_z|J_g^\mp J_g\rangle = \sqrt{\frac{J_g(2J_g+1)}{(J_g+1)}}\sum_{j,\lambda,\lambda'}(-1)^{j+\lambda'+J_g+1}D^{\lambda}_{J_g^\pm,j}D^{\lambda'}_{J_g^\mp,j}\left\{\begin{array}{ccc}\lambda & \lambda' & 1\\ J_g & J_g & j\end{array}\right\}\langle\lambda\|S\|\lambda'\rangle, \tag{21}$$

where the sum over λ and λ' is reduced to one term with $\lambda^\pi=2^+$ and $\lambda'^\pi=3^-$. Specifically, the matrix element of the Schiff operator between the quadrupole and octupole phonon states has the following form in terms of the RPA amplitudes (13):

$$\langle 2^+|S|3^-\rangle = \sqrt{35}\sum_{j_1,j_2,j_3}v^{(-)}_{j_1,j_2}\langle j_1\|S\|j_2\rangle\left\{\begin{array}{ccc}2 & 3 & 1\\ j_1 & j_2 & j_3\end{array}\right\}(A^{(2+)}_{j_2j_3}A^{(3-)}_{j_3j_1}+B^{(2+)}_{j_2j_3}B^{(3-)}_{j_3j_1}). \tag{22}$$

The results of the calculations are shown in Table I.

The matrix element of the first term of the interaction in Eq. (4) gives a dominant contribution that may be represented as

$$\langle ab;J^\pm M|W|cd;J^\mp M\rangle = \frac{G}{\sqrt{2}}\frac{1}{2m_p}\eta\,\langle ab;J^\pm M|W_1|cd;J^\mp M\rangle, \tag{23}$$

where

$$\langle ab;J^\pm M|W_1|cd;J^\mp M\rangle = F_1(abcd)\cdot K_1(ab;cd;J)+F_0(abcd)\cdot K_0(ab;cd;J) \tag{24}$$

for the interaction in the proton-neutron channel, while for the neutron-neutron channel it is given by

$$\langle ab;J^\pm M|W_1|cd;J^\mp M\rangle = \frac{K_0(ab;cd;J)}{\sqrt{(1+\delta_{ab})(1+\delta_{cd})}}\left[F_0(ab;cd)-(-1)^{J-j_c-j_d}F_0(ab;dc)\right]. \tag{25}$$

TABLE I: Calculated structure of the wave functions and the matrix element of the Schiff operator. The dominant quasiparticle and quasiparticle-phonon components for the ground state (J^π) and the first excited state ($J^{-\pi}$) of opposite parity are shown.

Nucleus	Structure						$\langle J^\pi J \vert S_z \vert J^{-\pi} J\rangle$
	J^π	$q.p.$	$q.p. \otimes \lambda^\pi$	$J^{-\pi}$	$q.p.$	$q.p. \otimes \lambda^\pi$	(e fm^3)
$^{217}_{88}$Ra$_{129}$	$9/2^+$	(82%) $g_{\frac{9}{2}}$	(10%) $[g_{\frac{9}{2}} \otimes 2^+]$	$9/2^-$	(0.01%) $h_{\frac{9}{2}}$	(0.01%) $[f_{\frac{5}{2}} \otimes 2^+]$	0.47
			(5%) $[j_{\frac{15}{2}} \otimes 3^-]$			(99%) $[g_{\frac{9}{2}} \otimes 3^-]$	
$^{217}_{86}$Rn$_{131}$	$9/2^+$	(77%) $g_{\frac{9}{2}}$	(12%) $[g_{\frac{9}{2}} \otimes 2^+]$	$9/2^-$	(0.02%) $h_{\frac{9}{2}}$	(0.01%) $[f_{\frac{5}{2}} \otimes 2^+]$	0.69
			(6%) $[j_{\frac{15}{2}} \otimes 3^-]$			(99%) $[g_{\frac{9}{2}} \otimes 3^-]$	
$^{219}_{88}$Ra$_{131}$	$7/2^+$	(5%) $g_{\frac{7}{2}}$	(85%) $[g_{\frac{9}{2}} \otimes 2^+]$	$7/2^-$	(0.4%) $f_{\frac{7}{2}}$	(0.3%) $[p_{\frac{3}{2}} \otimes 2^+]$	1.80
			(0.04%) $[h_{\frac{11}{2}} \otimes 3^-]$			(99%) $[g_{\frac{9}{2}} \otimes 3^-]$	
$^{219}_{86}$Rn$_{133}$	$5/2^+$	(25%) $d_{\frac{5}{2}}$	(64%) $[g_{\frac{9}{2}} \otimes 2^+]$	$5/2^-$	(1.2%) $f_{\frac{5}{2}}$	(0.24%) $[p_{\frac{1}{2}} \otimes 2^+]$	1.37
			(0.6%) $[h_{\frac{11}{2}} \otimes 3^-]$			(98%) $[g_{\frac{9}{2}} \otimes 3^-]$	
$^{221}_{88}$Ra$_{133}$	$5/2^+$	(33%) $d_{\frac{5}{2}}$	(57%) $[g_{\frac{9}{2}} \otimes 2^+]$	$5/2^-$	(2.3%) $f_{\frac{5}{2}}$	(0.6%) $[p_{\frac{1}{2}} \otimes 2^+]$	2.21
			(1.0%) $[h_{\frac{11}{2}} \otimes 3^-]$			(95%) $[g_{\frac{9}{2}} \otimes 3^-]$	
$^{221}_{86}$Rn$_{135}$	$7/2^+$	(18%) $g_{\frac{7}{2}}$	(22%) $[g_{\frac{9}{2}} \otimes 2^+]$	$5/2^-$	(0.7%) $f_{\frac{7}{2}}$	(0.2%) $[p_{\frac{3}{2}} \otimes 2^+]$	1.03
			(0.2%) $[j_{\frac{13}{2}} \otimes 3^-]$			(99%) $[g_{\frac{9}{2}} \otimes 3^-]$	
$^{211}_{86}$Rn$_{125}$	$1/2^-$	(91%) $p_{\frac{1}{2}}$	(5%) $[f_{\frac{5}{2}} \otimes 2^+]$	$1/2^+$	(0.2%) $s_{\frac{1}{2}}$	(0.01%) $[d_{\frac{5}{2}} \otimes 2^+]$	0.16
			(0.4%) $[g_{\frac{7}{2}} \otimes 3^-]$			(99.7%) $[f_{\frac{5}{2}} \otimes 3^-]$	

The coefficients F_0 and F_1 in Eqs. (24) and (25) represent radial parts of the matrix elements,

$$F_1(ab;cd) = I_r(abcd)(s_a + s_b + s_c + s_d + 2), \tag{26}$$

$$F_0(ab;cd) = I_r(abcd)(s_a - s_b + s_c - s_d) + I_{ac}(bd) - I_{bd}(ac), \tag{27}$$

where

$$I_r(abcd) = \int R_a R_b R_c R_d r dr, \quad I_{ac}(bd) = \int [R_a R_c]' R_b R_d r^2 dr, \tag{28}$$

and $s_a = (l_a - j_a)(2j_a + 1)$. The angular J-dependent part of the two-body matrix element is given by the coefficients

$$K_0(ab;cd;J) = (-1)^{j_b - j_d + l_b + l_d} \Pi(abcd) \begin{pmatrix} j_a & j_b & J \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} j_c & j_d & J \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \tag{29}$$

and

$$K_1(ab;cd;J) = \Pi(abcd) \begin{pmatrix} j_a & j_b & J \\ \frac{1}{2} & \frac{1}{2} & -1 \end{pmatrix} \begin{pmatrix} j_c & j_d & J \\ \frac{1}{2} & \frac{1}{2} & -1 \end{pmatrix}. \tag{30}$$

where $\Pi(abcd) = \sqrt{(2j_a+1)(2j_b+1)(2j_c+1)(2j_d+1)}/8\pi$.

The final expression for the interaction matrix element between the states J_g^π and $J_g^{-\pi}$ may be represented as a sum of two contributions,

$$\langle J_g^\pi | W | J_g^{-\pi} \rangle = W_{q.p.} + W_{q.p. \otimes ph}. \tag{31}$$

The first item originates from the interaction of the quasiparticle with the even-even core,

$$W_{q.p.} = C_{j_a = J_g^\pi} C_{j_{-a} = J_g^{-\pi}} w(a,-a) + \sum_{\lambda,b,-b} D^\lambda_{J_g^\pi, j_b} D^\lambda_{J_g^{-\pi}, j_{-b}} w(b,-b), \tag{32}$$

where

$$w(a,-a) = \sum_{j_c,J} \frac{(2J+1)}{(2j_a+1)} W_{q.p.}(ac;-ac;J). \tag{33}$$

Here the two-quasiparticle matrix element $W_{q.p}(ac;-ac;J_{ac})$ is a combination of the antisymmetrized two-particle interaction matrix elements weighted with the occupation factors of the single-particle states,

$$W_{q.p.}(ab;cd;J) = U_0(ab;cd) \langle j_a j_b; J | W | j_c j_d; J \rangle^{as} + \tag{34}$$

$$\frac{\left[U_1(ab;cd) \langle j_a j_b^{-1}; J | W | j_c j_d^{-1}; J \rangle - (-1)^{j_c + j_d - J} U_2(ab;cd) \langle j_a j_b^{-1}; J | W | j_d j_c^{-1}; J \rangle \right]}{\sqrt{(1+\delta_{ab})(1+\delta_{cd})}},$$

where the notations are used $U_0(ab;cd) = u_a u_b u_c u_d + v_a v_b v_c v_d$, $U_1(ab;cd) = u_a v_b u_c v_d + v_a u_b v_c u_d$, $U_2(ab;cd) = u_a v_b v_c u_d + v_a u_b u_c v_d$, and the two-body matrix elements in the particle-hole channel are related to the ones in the particle-particle channel through the Pandya relation,

$$\langle j_a j_b^{-1}; J | W | j_c j_d^{-1}; J \rangle = (-1)^{j_a + j_b + j_d + j_c + 1} \times \tag{35}$$

$$\sum_{J_1} (2J_1 + 1) \begin{Bmatrix} j_a & j_b & J \\ j_c & j_d & J_1 \end{Bmatrix} \langle j_d j_a; J_1 | W | j_b j_c; J_1 \rangle.$$

The simplicity of the angular part of the interaction allows one to perform the summation over J in Eq. (33) analytically. The result for $w(a,-a)$ has the following form:

$$w(a,-a) = -\frac{1}{4\pi} \sum_{j_c} (2j_c+1) \left[I_{cc}(a,-a) + \frac{I_r(ac,-ac)(s_c+1) + I_{cc}(a,-a)}{\sqrt{1+\delta_{ac}+\delta_{-a,c}}} \right] v^{(+)}_{a,-a}. \tag{36}$$

TABLE II: Calculated energy difference between the J_g^π and closest $J_g^{-\pi}$ state of opposite parity ($\Delta E^{\rm th}_{+,-}$), single-particle ($W_{q.p.}$) and collective ($W_{q.p.\otimes ph}$) contributions to the total matrix element of the $\mathcal{PT}$-odd interaction, Eq. (30), and corresponding value of the Schiff moment, Eq. (19). The corresponding values of the atomic dipole moment $\mathrm{d}_{\rm atomic}$ calculated using relations between Schiff and dipole moments [29] are listed in the last column. Previous measurements of $\mathrm{d}_{\rm atomic}$ were performed for Hg and Xe where $S \sim 1$ and $\mathrm{d}_{\rm atomic} \sim 1$ in the same units.

Nucleus	J_g^π	$\Delta E^{\rm th}_{+,-}$	$W_{q.p.}$	$W_{q.p.\otimes ph}$	$S(J_g^\pi)$	$\mathrm{d}_{\rm atomic}$
		(keV)	($\eta \cdot 10^{-2}$eV)	($\eta \cdot 10^{-2}$eV)	($\eta \cdot 10^{-8}$ e$\cdot$ fm^3)	($\eta \cdot 10^{-25}$ e$\cdot$ cm)
$^{217}_{88}$Ra$_{129}$	$\frac{9}{2}^+$	1384	-5.9$\cdot 10^{-2}$	-2.3	-1.58	13.4
$^{217}_{86}$Rn$_{131}$	$\frac{9}{2}^+$	1296	7.9$\cdot 10^{-2}$	-3.1	-3.31	-10.9
$^{219}_{88}$Ra$_{131}$	$\frac{7}{2}^+$	433	3.6$\cdot 10^{-2}$	-8.1	-70.1	595.9
$^{219}_{86}$Rn$_{133}$	$\frac{5}{2}^+$	969	3.4$\cdot 10^{-2}$	-6.5	-18.5	-61.1
$^{221}_{88}$Ra$_{133}$	$\frac{5}{2}^+$	991	2.3$\cdot 10^{-2}$	-11.5	-51.7	439.5
$^{221}_{86}$Rn$_{135}$	$\frac{7}{2}^+$	567	7.9$\cdot 10^{-2}$	-4.3	-15.6	-51.5
$^{211}_{86}$Rn$_{125}$	$\frac{1}{2}^-$	2222	-2.6$\cdot 10^{-2}$	-1.6	-0.23	-0.8

The second term in Eq. (32) is due to the interaction of the odd quasiparticle with quadrupole and octupole phonons:

$$W_{q.p.\otimes ph} = \sum_{a,b,c,d,e,\lambda,\lambda'} (-1)^{j_a+j_c+\lambda+\lambda'+1} \left(A^{(\lambda)}_{j_b j_e} A^{(\lambda')}_{j_d j_e} + B^{(\lambda)}_{j_b j_e} B^{(\lambda')}_{j_d j_e} \right) D^{\lambda}_{J_g^\pi, j_a} D^{\lambda'}_{J_g^{-\pi}, j_c} \times \tag{37}$$

$$\left[\delta_{a,c}\delta_{j_b,j_d} w(b,-b) + \sum_{J12} \Lambda(J_{12}J_{12}\lambda\lambda') \begin{Bmatrix} j_b & j_a & J_{12} \\ J_g & j_e & \lambda \end{Bmatrix} \begin{Bmatrix} j_d & j_c & J_{12} \\ J_g & j_e & \lambda' \end{Bmatrix} W_{q.p.}(ab, cd; J_{12}) \right],$$

where $\Lambda(J_{12}J_{12}\lambda\lambda') = (2J_{12}+1)\sqrt{(2\lambda+1)(2\lambda'+1)}$. The results for the interaction matrix element and final calculated values of the Schiff moment are shown in Table II.

IV. DISCUSSION

We analyze here the results of calculations presented in a previous section. As seen from Eq. (19), there are three quantities determining the value of Schiff moment: an off-diagonal matrix element of the Schiff operator, $\langle J_g^{-\pi} M = J_g | S_z | J_g^\pi M = J_g \rangle$, a matrix element of $\mathcal{PT}$-violating interaction, $\langle J_g^\pi | W | J_g^{-\pi} \rangle$, and excitation energy of the admixed state of opposite parity, $E(J_g^\pi) - E(J_g^{-\pi})$. Let us discuss these quantities separately.

The off-diagonal matrix elements of the Schiff operator, see Table 1, are clearly correlated with the amplitudes of particle-plus-phonon components, Eq. (21). In all cases under consideration, the neutron $g_{9/2}$ orbital has lowest energy and produces dominant particle-quadrupole and particle-octupole amplitudes. In the case when the ground state has spin $J^{\pi} = 9/2^{+}$ (i.e., ^{217}Ra and ^{217}Rn), the single neutron quasiparticle $g_{9/2}$ orbital dominates the ground state wave function. However, here there is only a contribution of small quasiparticle-phonon components leading to a small total matrix element of the Schiff operator.

As soon as the ground state has a spin value different from the spin of the $g_{9/2}$ orbital, the particle-quadrupole phonon component becomes dominant for the ground state, and the matrix element grows. One may notice also that the Schiff matrix element increases with the mass number even if the quasiparticle-quadrupole- phonon component becomes smaller (e.g., ^{221}Ra vs. ^{219}Ra). This is caused by the enhancement of collectivity towards the middle of the shell, where, for example, the $^{222-224}$Ra isotopes have already well pronounced deformed structure. Thus, the matrix elements of the Schiff operator are sensitive to details of nuclear structure and under favorable conditions these matrix elements may be enhanced by a factor of two to four, as it was mentioned in Sec. II.

The next important ingredient to the Schiff moment is a matrix element of $\mathcal{PT}$-violating interaction $\langle J_g^{\pi}|W|J_g^{-\pi}\rangle$. We have split it into two parts, a single quasiparticle, $W_{q.p.}$, and collective, $W_{q.p.\otimes ph.}$, contributions shown in Table II. Since the amplitude of the single-quasiparticle component is quite small for the excited state of negative parity, see Table I, the $W_{q.p.}$ part is by two-three orders of magnitude smaller than the estimated single-particle value, $\eta A^{-1/3}$ eV (η·0.16 eV for $A = 221$, for example). Therefore the main contribution comes from collective quasiparticle-phonon components. The collective contribution to the interaction is correlated with the matrix element of the Schiff operator: stronger interaction corresponds to a larger off-diagonal matrix element of the Schiff operator. In most cases the interaction matrix element is suppressed compared to its single-particle estimate; similar observation has been reported [21] in the case of Skyrme-Hartree-Fock calculations for deformed nuclei. However, there is a combined enhancement of the numerator in Eq. (19) which may differ by a factor of 15 for neighboring isotopes, as, for example, ^{217}Ra and ^{219}Ra.

Finally, there is a third factor, excitation energy of the opposite parity state, that enters the expression for the Schiff moment in the denominator. Coupling of the positive parity quasiparticle to the octupole phonon results in the gap $\Delta E_{+,-}$ that is at least by a factor of four smaller than the gap between single-particle partners with the same spin and opposite parity. If there is the

same single-particle orbital (in our case $g_{9/2}$) coupled to quadrupole and octupole phonons, then the gap is closely correlated with the distance between the 2^+ and 3^- states: the smaller it is the smaller is the value of $\Delta E_{+,-}$ and the larger is the enhancement factor for the Schiff moment. The $\Delta E_{+,-}$ gaps obtained in the framework of the QRPA are shown in Table II. The calculations of the Schiff moment with these energies yield the maximum value of 70 $\eta 10^{-8} e\cdot \mathrm{fm}^3$ for ^{219}Ra and slightly smaller one, 52 $\eta 10^{-8} e\cdot \mathrm{fm}^3$, for ^{221}Ra. Unfortunately, experimental data for the negative parity states for the nuclei discussed here are rather scanty. However, there are candidates for the $5/2^-$ state in ^{221}Ra at 104 keV and 450 keV. If these states have needed nature, then the Schiff moment may be around 450 $\eta 10^{-8} e\cdot \mathrm{fm}^3$ and 100 $\eta 10^{-8} e\cdot \mathrm{fm}^3$, respectively. A similar situation exists for ^{219}Rn, where the $5/2^-$ candidate is 500 keV lower than the corresponding calculated $5/2^-$ state. Taking into account that we have used the QRPA in its simplest version, one may expect stronger enhancement revealed by more realistic calculations.

Another interesting example is ^{211}Rn (see Table I and II). The calculated Schiff moment in this case is even smaller than the estimated single-particle value. This is caused by the fact that the ground $J^\pi = 1/2^-$ state has almost pure single-particle $p_{1/2}$ nature, while the first excited $J^\pi = 1/2^+$ state is calculated to be a pure quasiparticle-phonon $f_{5/2} \otimes 3^-$ state. Furthermore, the 3^- state is predicted to be high (1.7 MeV) and almost non-collective. There is no chance to get here any enhancement of the Schiff moment along the lines of our calculations. The coupling of the quasiparticle to other low-lying negative parity states may change the result although keeping the value on the same order of magnitude. The main contribution in this case is due to the polarization of the proton charge density in the core by the $\mathcal{PT}$-odd field (4) of the external neutron, the same mechanism that produces the Schiff moment of ^{199}Hg [27]. Therefore, $S(^{211}\mathrm{Rn}) \sim S(^{199}\mathrm{Hg})$, and $d_{\mathrm{atomic}}(^{211}\mathrm{Rn}) \sim d_{\mathrm{atomic}}(^{199}\mathrm{Hg})$.

V. CONCLUSION

To conclude, we have calculated the nuclear Schiff moment in nuclei known as relatively soft with respect to the octupole and quadrupole excitation modes. We found a considerable enhancement of the average magnitude comparable to what was found for nuclei having static octupole deformation. Among factors which contribute to this enhancement, the main role is played by small energy intervals between the opposite parity states and by the large vibrational amplitude in soft nuclei. The details of structure of the quasiparticle-phonon states are also important.

Our analysis shows that the most favorable conditions can be provided by proximity of the

quadrupole 2^+ and octupole 3^- phonon states, large proton component of the phonon states and coupling of the same single-quasiparticle state to quadrupole and octupole phonons. We have considered only the lowest symmetric quadrupole phonon in the present paper. In the presence of few active protons and neutrons, there is a possibility of low-lying "mixed-symmetry" quadrupole phonon in vibrational nuclei that is known to be connected to the octupole 3^- phonon by a considerably stronger E1 strength than the symmetric lowest quadrupole phonon [30]. Therefore one may expect additional enhancement if the coupling to the "mixed-symmetry" phonon is taken into consideration.

The conventional core polarization effects are also important for getting a certain quantitative prediction, although they are not expected to lead to a significant amplification of the effect. In the future the full calculations taking into account on equal footing collective and single-particle effects, including the $\mathcal{PT}$-violating corrections to the vibrational modes and core polarization, are to be carried out. It is desirable to extend the studies to lighter nuclei $A \approx 100$ with pronounced octupole phonon states with more experimental data available. This may help to understand better the nuclear structure effects for the enhancement of the Schiff moment and to explore a possibility of the correlation between the calculated values of the Schiff moment and observed E1 or E3 strength.

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[1] R. Fleischer, Phys. Rep. **370**, 537 (2002).

[2] J.S.M. Ginges and V.V. Flambaum, Phys. Rep. **397**, 63 (2004).

[3] M.V. Romalis, W.C. Griffith, J.P. Jacobs, and E.N. Fortson, Phys. Rev. Lett. **86**, 2505 (2001).

[4] J.P. Jacobs, W.M. Klipstein, S.K. Lamoreaux, B.R. Heckel, and E.N. Fortson, Phys. Rev. A **52**, 3521 (1995).

[5] V.V. Flambaum and G.F. Gribakin, Prog. Part. Nucl. Phys. **35** 423 (1995).

[6] J.J. Hudson, B.E. Sauer, M.R. Tarbutt, and E.A. Hinds, Phys. Rev. Lett. **89**, 023003 (2002).

[7] S.K. Lamoreaux, Phys. Rev. A **66**, 022109 (2002).

[8] T.N. Mukhamedjanov and O.P. Sushkov, physics/0411226.

[9] V.V. Flambaum, I.B. Khriplovich, and O.P. Sushkov, J. Exptl. Theor. Phys. **87**, 1521 (1984) [JETP **60**, 873 (1984)].

[10] V.V. Flambaum and O.K. Vorov, Phys. Rev. C **49**, 1827 (1994).

[11] V.F. Dmitriev and R.A. Sen'kov, Yad. Fiz. **66**, 1988 (2003) [Phys. At. Nucl. **66**, 1940 (2003)].

[12] V.F. Dmitriev, R.A. Sen'kov, and N. Auerbach, nucl-th/040865.

[13] W.C. Haxton and E.M. Henley, Phys. Rev. Lett. **51**, 1937 (1983).

[14] O.P. Sushkov and V.V. Flambaum, Usp. Fiz. Nauk **136**, 3 (1982) [Sov. Phys. Usp. **25**, 1 (1982)].

[15] G.E. Mitchell, J.D. Bowman, S.I. Pentila, and E.I. Sharapov, Phys. Rep. **354**, 157 (2001).

[16] O.P. Sushkov and V.V. Flambaum, Yad. Fiz. **31**, 55 (1980) [Phys. At. Nucl. **31**, 55 (1980)].

[17] V.V. Flambaum and V.G. Zelevinsky, Phys. Lett. B **350**, 8 (1995).

[18] V. Spevak and N. Auerbach, Phys. Lett. B **359**, 254 (1995).

[19] N. Auerbach, V.V. Flambaum, and V. Spevak, Phys. Rev. Lett. **76**, 4316 (1996).

[20] V. Spevak, N. Auerbach, and V.V. Flambaum, Phys. Rev. C **56**, 1357 (1997).

[21] J. Engel, M. Bender, J. Dobaczewski, J.H. de Jesus, and P. Olbratowski, Phys. Rev. **68**, 025501 (2003).

[22] J. Dobaczewsky and J. Engel, nucl-th/0503057, accepted to Phys. Rev. Lett.

[23] J. Engel, J.L. Friar, and A.C. Hayes, Phys. Rev. C **61**, 035502 (2000).

[24] V.V. Flambaum and V.G. Zelevinsky, Phys. Rev. C **68**, 035502 (2003).

[25] K. Kaneko, M. Hasegawa, and T. Mizusaki, Phys. Rev. C **66**, 051306(R) (2002).

[26] J. Armstrong and V. Zelevinsky, Preprint MSUCL-1125, April 1999; BAPS **44** (1999) 397.

[27] V.V. Flambaum, I.B. Khriplovich and O.P. Sushkov, Nucl. Phys. **A449**, 750 (1986).

[28] V.G. Soloviev, *Theory of Atomic Nuclei: Quasiparticles and Phonons* (IOP Publishing, Bristol, 1992).

[29] V.A. Dzuba, V.V. Flambaum, and J.S.M. Ginges, Phys. Rev. A **61**, 062509 (2000); V.A. Dzuba, V.V. Flambaum, J.S.M. Ginges, and M.G. Kozlov, Phys. Rev. A **66**, 012111 (2002).

[30] N. Pietralla, C. Fransen, A. Gade, N. A. Smirnova, P. von Brentano, V. Werner, and S. W. Yates, Phys. Rev. C **68**, 031305(R) (2003).